

Detection of Blockage Degree and Removing Strategies in Microreactor

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Abstract: Blockage is a common problem for microreactors, and the blockage degree directly affects the removing operation. In this work, the blockage degree is first defined as the ratio of the blocking volume over the volume of mixing channel based on computational fluid dynamics (CFD) models of different blockage types. After analyzing the limitation of this standard index, a new blockage index is proposed, in which the blocking volume, the cross-sectional area and the roughness of the blocking body are all taken into account. The relationship between the pressure difference and the new index is obtained through regression of CFD data to determine the blocking degree. Meanwhile, the classification of the removing blockage is also defined. The smaller the blockage index value is, the more difficult it is to remove the blockage. A inlet angle is introduced as a new design factor in choosing removing options.

Keywords: microreactor, blockage degree, blockage index, computational fluid dynamics (CFD) models; removing blockage.

1. INTRODUCTION

Microreactors offer advantages to chemical processing including good control of reaction time, provision of high interfacial area among phases for multiphase reaction systems, efficient heat management and optimum temperature control from reduced length scales. The low hold-up in a microsystem can offer controllability, reduced safety risks and lower environmental impact. The above features make microreaction devices particularly suitable for reactions which are highly exothermic and have short contact time. Meanwhile microreactors can also be employed as useful tools for process development that can not only facilitate process optimization, but also reduce the lag-time between laboratory development and industrial production (Chen et al., 2013; Luo et al., 2009).

The risk of being blocked is increased by twisted forces that include the interfacial tension, the liquid-solid surface tension, the viscous force and other surface forces in the microchannel (Cui et al., 2012; Zughbi et al., 2003). For example, in the process of micro-particles, the blockage is mainly caused by the intermolecular van der Waals force. If the temperature, the flow rate and the mixing state of the reaction process are not controlled well, the process of adhesion, aggregation and deposition are likely to form microchannel blockage (Mala et al., 1997).

Blockage in microreactors causes poor uniformity in the residence time distribution among microreactors and degrades product quality. Therefore, a blockage detection system is indispensable. Data-based and model-based blockage detection systems are developed to identify a blockage in stacked microreactors from the output signals of

temperature changes (Kano et al., 2007). A pressure balance model is proposed to locate channel blockage and estimate the degree of blockage (Yamamoto et al., 2009). The effects of sensor location and sensor number on the proposed blockage detection system are investigated based on an optimal designed distributor (Tanaka et al., 2011). The above blockage diagnosis systems are useful to cope with abnormal situations in which the blockage only occurs in one microreactor. A data-based blockage diagnosis system is proposed that can identify blockage in two microreactors by using pressure sensors (Noda, 2010). When a blocked microreactor is identified, it can be replaced with a new one to allow continued production. Tonomura et al. developed an effective operation and control method for parallelized microreactors to keep the flowrates at a desired value even when blockage occurs (Tonomura et al., 2008).

There are two kinds of blockage in microreactors: total blockage and partial blockage. For a total blockage condition, there is no reaction yield when faults occur, and the blockage can be detected by ΔP , the pressure difference between the inlet and the outlet (Tanaka et al., 2011; Wang et al., 2016). Under a partial blockage, the yield quality is decreased, and the reaction residence time is also changed. Meanwhile, unexpected reaction by-products cause waste of raw materials and economic losses. The above detection methods are all based on total blockage conditions. Very little work has been reported on how to deal with partial blockage in microreactors. This is mainly because the detection of partial blockage is rather difficult due to the small change in ΔP (Ho and Tai, 1998). Removing partial blockage is more cost-effective than replacing a totally blocked microreactor. However, the blockage degree needs to be determined before

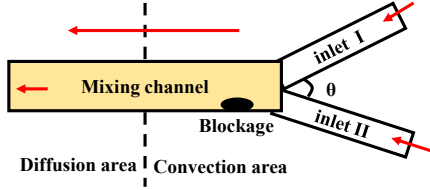


Fig. 1 Illustration of a Y-type microreactor.

it is removed because this affect the choice of removing strategies. In this work, we aim to develop effective methods to detect partial blockage faults for microreactor systems, based on which design removing strategies.

The rest of the paper is organized as follows. In Section 2, different blockage body structures are briefly introduced. Then in Section 3, a blockage index is proposed to classify the blockage degree, and a detailed detecting procedure is described. In Section 4, the classification of the removing blockage is defined accordingly. The inlet angle and the blockage location are designed to remove blockages. Conclusions are given in Section 5.

2. MODEL OF BLOCKAGE DEGREE

In this study, a blockage index is presented to define the removing difficulty, and blockage removing strategies are also analyzed by using this index.

2.1 Blockage Types

A Y-type microchannel with circular cross section is considered in this work as shown in Fig. 1. Blockage only exists in the mixing channel, therefore, the inlet part of the Y-type microreactor is ignored to start with.

Blockage is divided into two types along the flow direction as shown in Fig. 2: rough enhanced block (Fig. 2 (I)) and smooth block (Fig. 2 (II)). Two parameters are used to describe these two blockages: the block volume (V_b); and the tangential surface area (S_L) that is in contact with the reaction fluid. The cross section of a partial blockage can be divided into three types: circular, square and triangular section blocks (see Fig. 2 (III) ~ (V)). The parameters to describe these blockages are: V_b and the block surface area (S_v), which is perpendicular to the reaction fluid.

The main purpose of determining the blocking degree is to evaluate the methods of removing blockage. According to the above classifications, the block is more easy to remove if V_b is smaller, S_v is greater and S_L is smaller (a rough surface), for the block is a paper-like structure, that is thin and flat. On the other hand, if S_v is small, which means that the block body spreads the channel surface, and S_L is greater (a smooth surface), then removing the blockage is relatively difficult.

2.2 Blockage Degree

In the microchannel, a total blocking means that the flow rate is 0, and partial blocking means that the flow rate is reduced

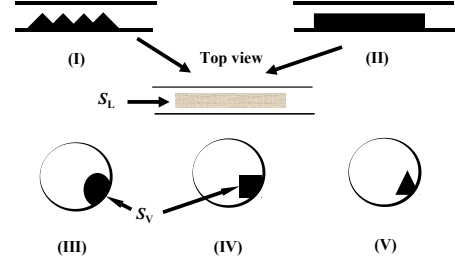


Fig. 2. Different blockage types in a microreactor

but not to zero, therefore, the blockage degree is defined by a measure of flow rate reduction.

When the channel length L and the diameter D are constant, the change in the flow rate can be obtained by (Cao, 2013)

$$u = C\sqrt{RJ} \quad (1)$$

Herewith: u is the average flow rate, R is the hydraulic diameter ($= D/4$), the coefficient C is defined as:

$$C = \sqrt[6]{R/n} \quad (2)$$

Herewith: n is the roughness of the channel. When the channel is placed horizontally, the hydraulic gradient J is related to ΔP by

$$J = \Delta P / (\rho g L) \quad (3)$$

L , D and the solution density ρ of a microreactor are constant in (1)-(3). The factor that affect the flow rate change is ΔP and n . If n is ignored, it is assumed that the block is smooth, as shown in Fig. 2 (II). The degree of u reduction is only calculated by.

In the blockage condition, ΔP is increased in order to keep a constant u , and the volume of reactant is decreased. Therefore, the blockage degree is defined as:

$$RV = V_b / V \quad (4)$$

where V is the volume of the mixing channel. The relationship between ΔP and RV is analysed next.

A CFD model under non-blocking condition is established on ANSYS. The unstructured meshing of the mixing channel part of the Y-type microreactor (no-inlet part) is carried out by using a given L and D in ICEM. The meshed grid is imported into FLUENT. The laminar flow model is selected, and the input flow rate u and atmospheric pressure outlet are set. In this study, the microchannel is made of stainless steel, the reaction solution is water, and the first order upwind algorithm is used to solve N-S equations. The ΔP is calculated from the CFD model and defined as a baseline reference, ΔP_b .

Then a CFD model for blockage type (II) + (III) is established and shown in Fig. 3, the shadow part in the channel is a blockage, that is, a smooth block with the circular section. By changing V_b , ΔP is also changed. Then the relationship between ΔP and RV can be determined.

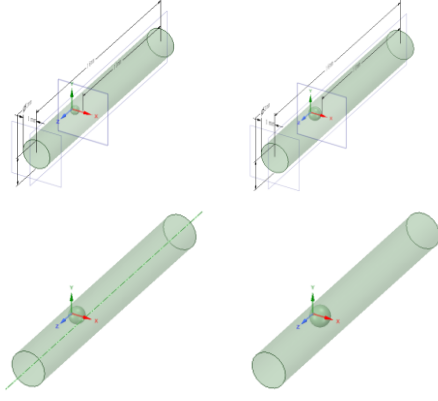


Fig. 3. Smooth block with circular cross section.

Table 1. A case study of ΔP and RV in circular cross section with $L=16$ mm, $D=2000$ μm , $u=1\text{m/s}$.

RV	ΔP	λ
0	ΔP_b	1
0.005	$1.24\Delta P_b$	1.24
0.01	$1.64\Delta P_b$	1.64
0.04	$2.47\Delta P_b$	2.47
0.05	$5.11\Delta P_b$	5.11

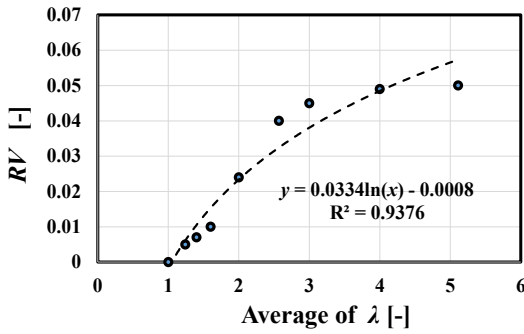


Fig. 4. Relationship between RV and λ .

Table 1 gives an example under constant L , D and u . ΔP is described as $\Delta P = \lambda \Delta P_b$, and is also listed in Table 1. Fig. 4 depicts the correspondence between the change of ratio λ and the RV :

$$RV = a \ln(\lambda) - b \quad (5)$$

where the parameters are fitted to be $a = 0.034$ and $b = 0.008$. For a real Y-type microreactor, ΔP_b is first measured under the normal operation condition. If ΔP_b is changed to ΔP , then λ is calculated, and RV is determined. A large value of RV means a larger degree of blockage.

A blockage of the type (II) + (IV) is then simulated, as shown in Fig. 5, that is, the blockage with a square section. Following the similar procedure above, the relationship between λ and RV is investigated. When V_b changes by 5 times, ΔP remains almost unchanged. Therefore, the relationship shown in (4) cannot be used to determine the degree of blocking by measuring ΔP . A new definition of blockage degree is indispensable.

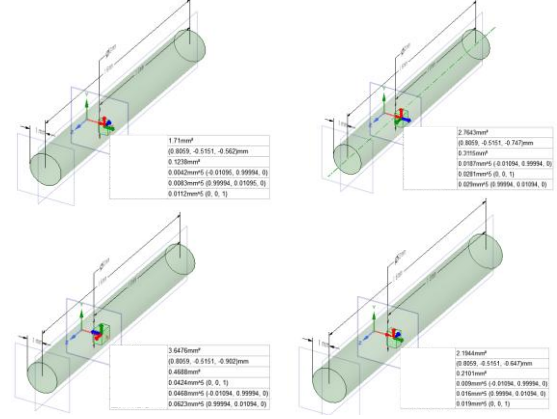


Fig. 5. Solid block with rectangular cross section.

From the analysis on the effect of two different partial blockages, it can be observed that the circular cross-section surface is smoother and the resistance to fluid is smaller, while the square cross section has larger influence on the fluid flow due to its angle characteristics. In the above discussion, on the blockage degree, the influence of the roughness n in is ignored. In practice, however, the blockage causes the growth in n to some extent, which should be considered in the evaluation of the blockage degree.

3. BLOCKAGE INDEX

Considering the blockage type I in Fig. 2, the surface roughness increases as compared to type II, and this increase in roughness can be described by its blocking characteristic parameter, S_L . With different cross-sections of the blocking types (III~V), S_V is indispensable to calculate the blockage degree. Therefore, an alternative blockage index is proposed as

$$A = \frac{S_V}{S_L} \frac{V_b}{V} \quad (6)$$

There are two main features of this new blockage index described in the following.

(i) When the surface area ratio of S_V/S_L is constant, the main factor affecting A is the volume of the blocking body, V_b . The smaller V_b is, the larger A is, and the lower the degree of blockage is.

(ii) When V_b is constant, a larger S_V/S_L ratio means the blockage surface is more rough. The cross-sectional area is large, and the impact on the blockage is large too. Therefore, A is larger as well.

Based on the calculations results of ΔP in Fig. 3 and Fig. 5, a CFD model of blockage types in Figs. 6-7 is added. Fig. 6 shows different S_V blocking situations under the same V_b , and Fig. 7 shows different S_L blocking situations when V_b and S_V are the same. Different S_L is assumed corresponding to different cross-sectional structure: oval, square and triangle.

Table 2 lists the calculation results of ΔP in Fig. 7. ΔP is also described as $\Delta P = \lambda \Delta P_b$. Meanwhile, Fig. 8 depicts the relationship between the change of λ and A :

$$A = c_2 \lambda^2 - c_1 \lambda + c_0 \quad (7)$$

where the coefficients are fitted to be $c_2 = 3.8757$, $c_1 = 6.6821$ and $c_0 = 17.39$.

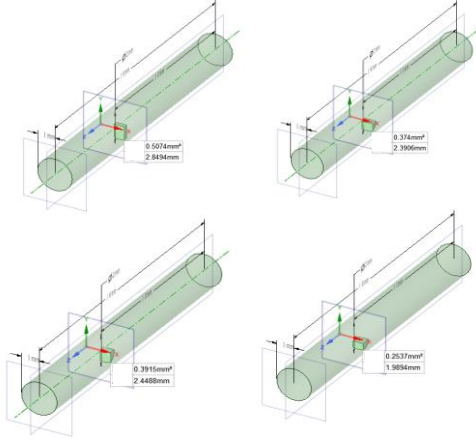


Fig. 6. Square blocks with the same V_b and different S_v .

Table 2. A case study of ΔP and RV with $L=16$ mm, $D=2000$ μm , $u=1$ m/s.

TYPE	ΔP		
	$(RV=0.002, S_{v1}=0.20D^2)$	$(RV=0.004, S_{v1}=0.26D^2)$	$(RV=0.008, S_{v1}=0.32D^2)$
oval	$1.01\Delta P_b$	$1.26\Delta P_b$	$1.28\Delta P_b$
square	$1.15\Delta P_b$	$1.31\Delta P_b$	$1.39\Delta P_b$
triangular	$1.21\Delta P_b$	$1.48\Delta P_b$	$1.50\Delta P_b$

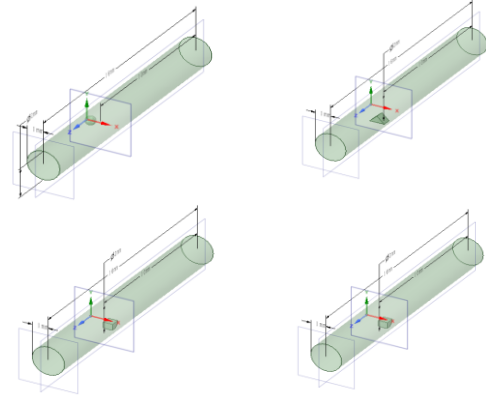


Fig. 7. Solid blocks with same V_b , S_v and different S_L .

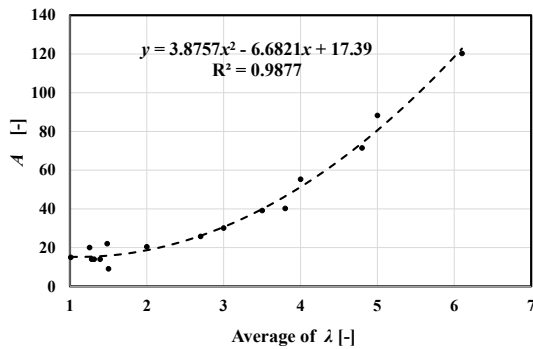


Fig. 8. Relationship between A and λ .

For a real Y-type microreactor, if a blockage fault is occurred, ΔP_b is changed to a new value, then λ is calculated, and A is determined by (7). The larger is the value of A , the higher is the degree of blockage.

The blockage index A can also indicate the difficulty of removing the blockage. The impact force of the blocking body's cross-section, f , can be calculated in the CFD model, and then the corresponding A value can be obtained. In this simulation, $f_b = 0.14$ N is set to be the base force when $A = 30$. Under different values of A , the force is calculated and listed in Table 3. The third column in Table 3 is the difficulty level of removing the blockage. "1" means most easy to remove, while "5" means most difficult to remove. The explanations are as follows:

(i) When V_b is constant in (6), if A is large, then S_v is large, f is large, and therefore, increasing the flow rate is the first choice to remove the blockage.

(ii) When S_v is constant in (6), if A is small, then V_b is large, which indicates that there are more block bodies spread among the mixing channel surface, so increasing the flow rate is not a suitable way to remove the blockage. Some other methods need to be applied.

Table 3. Relationship between A and the difficulty of blockage moving.

A	the force of cross-section	difficulty of removing the blockage
120	$42f_b$	1
55	$9f_b$	2
30	f_b	3
20	$0.7f_b$	4
15	$0.14f_b$	5

4. DESIGN OF REMOVING STRATEGY BASED ON INLET ANGLE

If the blockage is located at the front part of the mixing channel, in addition to increasing the flowrate, the inlet angle, θ (see Fig. 1), which affect the magnitude of the impact force on the inner surface of the mixing channel, can also be designed in order to improve removing of blockages.

The best mixing effect is obtained when $\theta=45^\circ$ in the case of the best flow ratio (inlet I flowrate/inlet II flowrate) (Liu et al., 2013; Squires and Quake, 2005). However, $\theta=45^\circ$ is the most unfavorable design for the blockage removing because of the minimum pressure gradient on the channel wall (Lin, 2008; Wu, 2011).

4.1 Study based on CFD

Assuming $A=15$, which indicates the most difficult situation to remove the blockage, the impact force f is calculated for $\theta=30^\circ$ and $\theta=60^\circ$, respectively. The block is assumed to be at the front of the channel ($0.9L$, close to the inlet). The simulation results are shown in Fig. 9 and Fig. 10. Based on the surface pressure of the block, $f=8.22f_b$ when $\theta=60^\circ$, and

$f=0.94f_b$ when $\theta=30^\circ$, the impact force on the blockage is larger with $\theta=60^\circ$ than with $\theta=30^\circ$. Therefore it is easier to remove the blockage when $\theta=60^\circ$.

4.2 Study based on Mechanistic Model

Furthermore, the impact force on the blockage is calculated by first-principle models in order to verify the CFD results. Under the microscopic condition, the interaction between molecules mainly includes the van der Waals force, the electrostatic force and spatial displacement force. Although the basic force between molecules is essentially the short-range force, but its accumulation effect can lead to greater effect than that of the $1\mu\text{m}$ long-range force. In order to facilitate the calculation, the long-range forces are used to calculate the impact force in this study without using any short-range force (Liu, 2011).

The blockage in the channel is equivalent to an immobile particle with a diameter of 0.33 mm. The force of the blockage is analyzed in the following at the angle of 30° and 60° .

- (i) Effective gravity force F_g : the effective gravity of the blockage is indispensable because the size of the equivalent particle is not negligible to the microchannel.

$$F_g = \frac{1}{6} \pi d_s^3 (\rho_s - \rho_w) g \quad (8)$$

Here d_s is the diameter of the equivalent particle, ρ_s and ρ_w are densities of the particle and the solution, respectively.

- (ii) Drag force of the flow, F_D : this impact force on the blockage is:

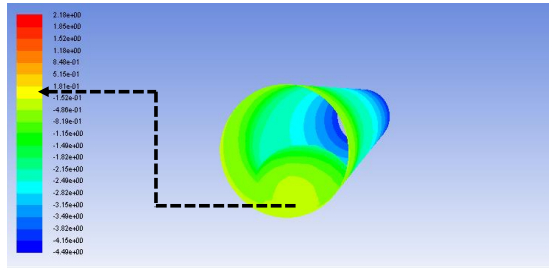


Fig. 9. The blocking surface pressure at $\theta=60^\circ$ from CFD calculation.

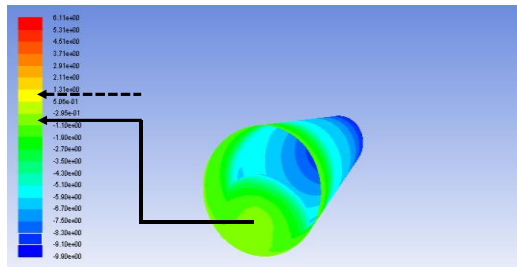


Fig. 10. The blocking surface pressure at $\theta=30^\circ$ from CFD calculation.

$$F_D = C_D \cdot \frac{1}{8} \pi d_s^2 \rho_w (u_w - u_s)^2 \quad (9)$$

Here u_s and u_w are the flow rate of particle and solution respectively. $u_w = 2 u_{in} \cos(\theta/2)$, u_{in} is the inlet flow rate of the Y-type microreactor. The resistance coefficient C_D is related to the Reynolds number:

$$\begin{cases} C_D = \frac{24}{Re} & Re < 1 \\ C_D = \frac{30}{Re^{0.625}} & 1 < Re < 1000 \end{cases} \quad (10)$$

$$Re = \frac{\rho_s d_s |u_w - u_s|}{\mu} \quad (11)$$

where μ is the dynamic viscosity of the solution. When the particles sink in the solution, the liquid gives the particles an upward force. However, this lift force for the blockage is very small, and it can be omitted. Then, the friction force of the blockage, F_f , which is in the opposite direction of F_D , that is

$$F_f = \eta F_g \quad (12)$$

where η is the friction coefficient, and it is 0.15 if the equivalent blockage particle and the microchannel are considered as two rigid bodies.

The drag force combined with the friction force composes the impact force in the flow direction on the blockage. If the blockage is stationary, then $u_s = 0$ and $F_f > F_D$. Therefore, the impact force is about equal to F_D . According to the value of u_w at the inlet angle of 30° and 60° , respectively, the $F_D^{60^\circ} = 9.5 F_D^{30^\circ}$, that is, when $\theta=60^\circ$, the impact force is 9.5 times of that of $\theta=30^\circ$, which is close to the CFD calculation relation (in Section 4.1, $8.22/0.74 = 8.7$). This result indicates that changing the inlet angle can effectively improve the impact force on the blockage, and therefore remove the blockage more easily.

The blockage discussed above is assumed to be in the front part of the mixing channel, i.e., the convection area in Fig. 1. It is the main reaction region where the channel is blocked. Whether the blockage location is in the convection area (near inlet) or in the diffusion area (near outlet), its effect can be analyzed by the comparison of ΔP changes.

A Y-type microreactor with the inlet angle of 60° and at different blocking positions are studied as an example. The blockage index A is set to be 30, which indicates the middle level of difficulty to remove the blockage. ΔP calculated under non-blocking condition is taken as the baseline reference, denoted as ΔP_b^Y . The calculation results are listed in Table 4. A factor β is introduced to describe the blocking position, as shown in Fig. 11. The data in Table 4 shows that the flow patterns produce a large fluctuation if the blockage is near the outlet. In this case, ΔP changes a lot, therefore it is a good option to increase the flowrate to remove the blockage. If the blockage is located near the convective zone, the fluid tends to be stable after a long distance from the blockage, and ΔP is lower than that in the diffusion area. In the latter case, a proper design of the inlet angel is a better option to remove the blockage rather than increasing the flowrate.

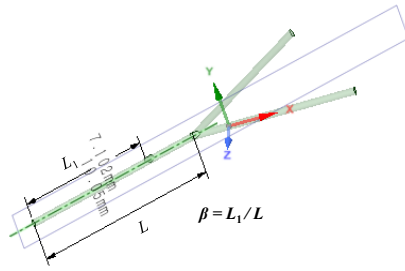


Fig. 11. Description of blocking position in a Y-type microreactor

Table 4. A case study of ΔP and blocking position with $L=10$ mm, $D=2000$ μm , $u_{\text{in}}=0.58$ m/s

β	ΔP ($\theta=60^\circ$)
Unblocked	ΔP_b^{YI}
0.12	$2.96 \Delta P_b^{\text{YI}}$
0.30	$2.98 \Delta P_b^{\text{YI}}$
0.38	$2.98 \Delta P_b^{\text{YI}}$
0.51	$2.95 \Delta P_b^{\text{YI}}$
0.60	$2.93 \Delta P_b^{\text{YI}}$
0.72	$2.94 \Delta P_b^{\text{YI}}$
0.80	$2.94 \Delta P_b^{\text{YI}}$
0.90	$2.92 \Delta P_b^{\text{YI}}$

5. CONCLUSIONS

In this study, the blockage degree of different types of partial blockage in the Y-type microreactor is discussed. A quantitative blockage index is proposed based on CFD models and numerical fittings. With this new index, the difficulty level of removing blockage in the microchannel can be determined.

The volume, the cross-sectional area of the blockage and the tangential area which denotes the roughness of the blockage are all considered in the proposed blockage index. Using the measured pressure difference, the blockage index can effectively indicate the blockage degree. In the future work, the temperature effect of the reaction in the microreactor, can also be considered to determine the blockage degree.

In addition, this paper analyzes the effect of inlet angle on the removal of blockage in the Y-type microreactor. From numerical studies, it is proved that the inlet angle at 60° is more effective in removing the front blockage than the angle of 30° . In the next step of the research, an optimal design of the inlet angle will be further investigated.

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